

# Commensurate Supersolid of Three-Dimensional Lattice Bosons

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Using an unbiased quantum Monte Carlo method, we obtain convincing evidence of the existence of a checkerboard supersolid at a *commensurate* filling factor  $1/2$  (commensurate supersolid) in the soft-core Bose-Hubbard model with nearest-neighbor repulsions on a cubic lattice. In conventional cases, supersolids are realized at incommensurate filling factors by a doped-defect-condensation mechanism, where particles (holes) doped into a perfect crystal act as interstitials (vacancies) and delocalize in the crystal order. However, in the above model, a supersolid state is stabilized even at the commensurate filling factor  $1/2$  *without doping*. By performing grand canonical simulations, we obtain a ground-state phase diagram that suggests the existence of a supersolid at a commensurate filling. To obtain direct evidence of the commensurate supersolid, we next perform simulations in canonical ensembles at a particle density  $\rho = 1/2$  and exclude the possibility of phase separation. From the obtained snapshots, we discuss the microscopic structure and observe that interstitial-vacancy pairs are unbound in the crystal order.

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Since the observation of a nonclassical moment of inertia in solid  $^4\text{He}$  by Kim and Chan[1, 2], the possible existence of supersolid has been discussed intensively. Regarding the possibility of a bulk supersolid in  $^4\text{He}$ , Prokof'ev and Svistunov pointed out that, in the absence of symmetry between vacancies and interstitials, a commensurate supersolid in continuous space has zero probability of being observed in nature[3]. Thus, they suggested that another scenario should be considered to interpret the decrease in nonclassical rotational inertia observed in  $^4\text{He}$ . In contrast to the case of continuous spaces, the presence of supersolid states in lattice systems has been established by unbiased quantum Monte Carlo simulations[4–14], particularly in the case when particles are added to or removed from perfect crystals. As a result of recent progress in experiments on cold atoms and molecules, optical lattice systems have become highly promising systems for realizing the supersolid state. In conventional cases, we can call such a supersolid state an incommensurate supersolid state, because it is realized by doping defects such as interstitials or vacancies into perfect crystals.

Although a commensurate supersolid in continuous space has zero probability of being found in nature, this does not apply to systems with explicitly broken translational symmetry such as lattice systems[3]. Among the optical lattice systems, one of the most promising candidates for realizing a supersolid is a checkerboard-type supersolid near filling factor  $1/2$ , because it can be realized only in the presence of appropriate nearest-neighbor repulsions of soft-core bosons on simple square or cubic lattices[7, 11, 14]. Therefore, it is an interesting question whether such a checkerboard supersolid can be stabilized even at the commensurate filling factor  $1/2$  *in the absence of doping*. Regarding the soft-core extended Bose-Hubbard model with nearest-neighbor repulsions,

the mean-field analysis[11] and the Gutzwiller variational method[15, 16] predicted that a checkerboard supersolid is stabilized at the commensurate filling factor (particle density)  $\rho = 1/2$  in addition to above and below  $\rho = 1/2$ . In contrast to these studies, exact quantum Monte Carlo studies have found evidence of a supersolid phase only above  $\rho = 1/2$  in 1D and 2D systems[7, 8]. However, recent quantum Monte Carlo studies have revealed that a supersolid phase exists below  $\rho = 1/2$  as well as above  $\rho = 1/2$  in the case of a 3D cubic lattice[11, 14]. This is consistent with the prediction by the mean-field analysis and the Gutzwiller variational method, and also suggests the presence of a supersolid phase at  $\rho = 1/2$ . To obtain direct evidence of a supersolid existing at the commensurate density  $\rho = 1/2$ , it is necessary to consider the canonical ensemble at  $\rho = 1/2$  and exclude the possibility of a phase separation, neither of which have been investigated previously. In this Letter, using an unbiased quantum Monte Carlo method, we show convincing evidence of a commensurate supersolid existing in the above-mentioned 3D system. The finite-temperature transition to a commensurate supersolid is also investigated. Finally, we show snapshots of the commensurate supersolid and discuss a microscopic structure.

The model considered here is the soft-core Bose Hubbard model with nearest neighbor repulsions on cubic lattices. The Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) - \mu \sum_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_{\langle i,j \rangle} n_i n_j. \quad (1)$$

Here,  $b_i^\dagger (b_i)$  and  $n_i$  are the bosonic creation (annihilation) operator on site  $i$  and the particle number operator defined as  $n_i = b_i^\dagger b_i$ , respectively. Furthermore,  $t$ ,  $\mu$ ,  $U$ , and



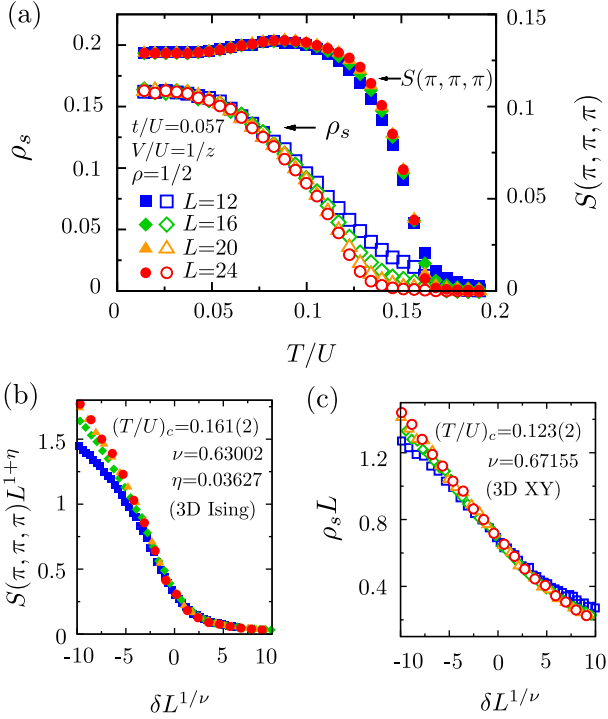


FIG. 3: (Color online) (a) Finite-temperature transition to the commensurate supersolid state. (b) Finite-size scaling of  $S(\pi, \pi, \pi)$  for the normal-to-CB transition. (c) Finite-size scaling of  $\rho_s$  for the CB-to-SS transition.

CB lobe. This result suggests the possible existence of commensurate supersolids, because we can expect that the system with a fixed density  $\rho = 1/2$  undergoes a phase transition from the CB solid state not directly to the SF state, but to the SS state as  $t$  increases. This can be also expected from  $\mu$  dependence of the measured quantities. In Fig. 2(c), the physical quantities at  $(t/U, V/U, T/t) = (0.057, 1/z, 0.3)$  are shown as functions of the chemical potential. As the chemical potential increases, the SF-to-SS transition occurs at  $\rho < 1/2$ , and the particle density increases to above  $\rho = 1/2$ . Since there is no insulating phase in which the particle density has a plateau and the superfluid stiffness vanishes, we expect that the SS phase remains even at  $\rho = 1/2$ . To explain this in more detail, we also show  $\rho_s$  and  $S(\pi, \pi, \pi)$  as functions of the particle density  $\rho$  in Fig. 2(d). These results are obtained by making bins for particle densities with a finite width and categorizing each sample into the appropriate bin. Although these results support the hypothesis that both finite  $\rho_s$  and  $S(\pi, \pi, \pi)$  survive at  $\rho = 1/2$ , we also have to exclude the possibility of a phase separation at exactly  $\rho = 1/2$ , to conclude the presence of a supersolid at the commensurate filling factor  $1/2$ .

To obtain direct evidence of the existence of a commensurate supersolid, we next perform simulations for  $\rho = 1/2$ . The following results were obtained by using only samples with  $\rho$  that is exactly equal to  $1/2$ . In other words, we performed quantum Monte Carlo calculations

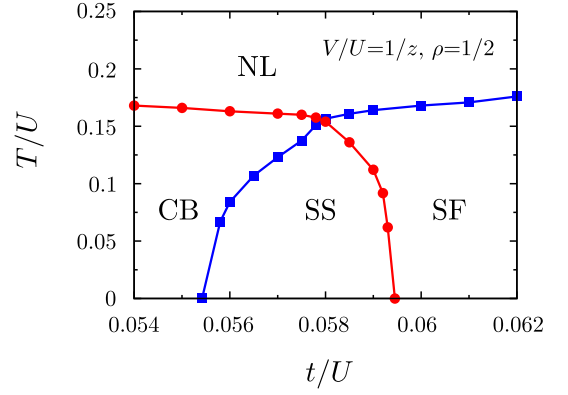


FIG. 4: (Color online) Finite-temperature phase diagram at the fixed density  $\rho = 1/2$ . Circles and squares denote the critical temperatures for the checkerboard order and superfluidity, respectively. The disordered phase at finite temperatures is referred to as normal liquid (NL) phase.

in a canonical ensemble at  $\rho = 1/2$ . In Fig. 3, the temperature dependences of  $\rho_s$  and  $S(\pi, \pi, \pi)$  are shown at  $(t/U, V/U) = (0.057, 1/z)$ . We can confirm finite values of  $\rho_s$  and  $S(\pi, \pi, \pi)$  at low temperatures. In our simulations,  $\rho_s$  and  $S(\pi, \pi, \pi)$  for all replicas, which were simulated under different initial conditions and with different seeds of random number, converged to the same values. This indicates the absence of a phase separation.

To clarify the existence of a finite-temperature transition to the commensurate supersolid state, we performed finite-size scaling analysis. Since the breaking symmetries in the supersolid state are  $Z_2$  and  $U(1)$ , which are related to the checkerboard order and the superfluidity, respectively, two successive transitions of the Ising-type universality class and the XY universality class are expected. We analyze the finite-size-scaling behavior of the structure factor and the superfluid stiffness by considering the scaling forms  $S(\pi, \pi, \pi)L^{1+\eta} = f(\delta L^{1/\nu})$  and  $\rho_s L = g(\delta L^{1/\nu})$ , respectively. Here,  $\delta$  is defined as  $\delta = (T - T_c)/T_c$ , and  $T_c$  is the critical temperature. Using the critical exponents of the 3D Ising universality class ( $\nu=0.63002$  and  $\eta=0.03627$ [23]) for the structure factor and the 3D XY universality class ( $\nu=0.67155$ [24]) for the superfluid stiffness, we successfully observed data collapses. As shown in Figs. 3(b) and (c), the data of system sizes larger than  $L \sim 16$  are necessary to obtain good scaling results. These results of finite-size scaling also strongly indicate the absence of a phase separation at  $\rho = 1/2$ . Therefore, we conclude that a true commensurate checkerboard supersolid exists in the present model. In Fig. 4, we summarize the transition points in the finite-temperature phase diagram at  $\rho = 1/2$ .

Finally, we discuss the microscopic structure of the commensurate supersolid. As discussed in Ref. [3], in the supersolid state, interstitials and vacancies do not form bound pairs and can be found arbitrarily far from each other. The delocalized defects give rise to superfluidity in crystal orders. In contrast, in the insulating

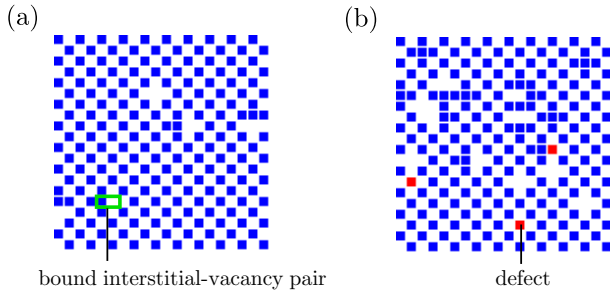


FIG. 5: (Color online) Cross-sectional snapshots at a fixed  $z$ -coordinate and imaginary time in  $N=20^3$  systems. (a) Checkerboard solid state at  $(t/U, V/U, T/U)=(0.052, 1/z, 0.02)$  and (b) commensurate supersolid state at  $(t/U, V/U, T/U)=(0.056, 1/z, 0.02)$ . Particle filling is exactly  $\rho = 1/2$  in both cases, although this cannot be confirmed from a single cross section above. Sites are denoted as rectangles. Empty rectangles, blue rectangles, and red rectangles indicate empty sites, singly occupied sites, and doubly occupied sites, respectively. In (a), the green rectangular frame represents a bounded interstitial-vacancy (particle-hole) pair confined within a nearest-neighbor site. In (b), the existence of several doubly occupied sites suggests the presence of interstitials and vacancies that are unbound beyond the nearest-neighbor sites.

phases, locally created particle-hole pairs are typically confined within nearest-neighbor sites, as has been well discussed for the Mott insulator at  $\rho = 1$ [25]. To qualitatively confirm the characteristic features, we show snapshots at the commensurate density  $\rho = 1/2$  in Fig. 5. In the checkerboard insulating phase [Fig. 5(a)], we observe bound interstitial-vacancy pairs that are typically

confined within nearest-neighbor sites. In contrast, in the commensurate supersolid state [Fig. 5(b)], we can easily observe interstitials and vacancies that are separated by a distance exceeding the nearest-neighbor distance. This can be confirmed from the presence of doubly occupied sites because such sites are never created from interstitial-vacancy pairs confined within nearest-neighbor sites. Since we did *not* dope any interstitials or vacancies into the commensurate solid, the defects originated from the unbound interstitial-vacancy pairs. In this sense, it is expected that the mechanism of the CB-to-SS transition is similar to the released doublon-holon mechanism of the MI-to-SF transition at  $\rho = 1$ [25].

In conclusion, using exact quantum Monte Carlo simulations, we obtained direct evidence of the existence of a checkerboard supersolid at  $\rho = 1/2$  in 3D bosonic systems. By obtaining a finite-temperature phase diagram at  $\rho = 1/2$ , we also showed the range of parameters in which this supersolid exists, including its temperature. Finally, from snapshots, we qualitatively discussed the its microscopic structure. Although the snapshots suggest the existence of unbound interstitial-vacancy pairs in the commensurate supersolid, further investigation is needed to confirm this quantitatively.

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